



# Evolution of in-cylinder polycyclic aromatic hydrocarbons in a diesel engine fueled with *n*-heptane and *n*-heptane/toluene



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## HIGHLIGHTS

- The evolutions of PAHs in the diesel engine combustion process were ascertained.
- PAHs with five-membered ring structure were abundant in combustion process.
- The evolutions of in-cylinder PAHs were varied after toluene addition.
- Toluene addition generally reduced the  $\Sigma M_{PAHs}$  during the combustion process.
- Toluene addition was conducive to the growth of PAHs to form larger PAHs.

## ARTICLE INFO

### Article history:

Received 29 January 2015

Received in revised form 21 May 2015

Accepted 22 May 2015

Available online 1 June 2015

### Keywords:

Diesel engine

Polycyclic aromatic hydrocarbon

Toluene

*n*-Heptane

Combustion process

## ABSTRACT

This work studied the evolution of in-cylinder polycyclic aromatic hydrocarbons (PAHs) in a diesel engine fueled with *n*-heptane, and explored the effects of adding toluene to *n*-heptane on in-cylinder PAHs. In-cylinder PAHs were sampled in a direct injection diesel engine using a total cylinder sampling system. PAHs were analyzed by gas chromatography–mass spectrometry with programmed temperature vaporization in the solvent vent mode. For *n*-heptane, the mass of total in-cylinder PAHs ( $\Sigma M_{PAHs}$ ) increased in premixed and late diffusion combustion phases, and decreased in early diffusion and late combustion phases. Among the 16 PAHs detected, Naphthalene (Nap) was the most abundant. PAHs with two benzene rings and one five-membered ring, such as Acenaphthylene, Acenaphthene and Fluorene, were also plentiful, implying that PAHs with five-membered ring could play an important role in the growth of in-cylinder PAHs. When adding 20 vol.% toluene to *n*-heptane, the evolution of  $\Sigma M_{PAHs}$  was varied. The  $\Sigma M_{PAHs}$  for *n*-heptane/toluene increased in premixed and early diffusion combustion phases, and decreased in late diffusion and late combustion phases. Toluene addition reduced the  $\Sigma M_{PAHs}$  in the premixed combustion phase by up to 48% but increased  $\Sigma M_{PAHs}$  by 30% in the early diffusion combustion phase. In the subsequent combustion phase, the  $\Sigma M_{PAHs}$  was reduced by approximately 67%. For in-cylinder individual PAHs, toluene addition generally reduced the percentages of Nap in  $\Sigma M_{PAHs}$  during the engine combustion process but increased the percentages of larger PAHs, indicating that toluene addition was conducive to the growth of PAHs to form larger PAHs.

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## 1. Introduction

Polycyclic aromatic hydrocarbons (PAHs) are key intermediates in soot formation [1–5]. In the soot nucleation process, for example, PAHs are considered to act as the building blocks that undergo chemical reactions to form incipient soot; in the soot surface growth process, they contribute to the growth of soot particles by attaching to soot outer surfaces. Because the PAH formation mechanism and the process by which PAHs are transformed to soot

are quite complex, the field of combustion research still has much to learn regarding PAHs and soot formation.

There has to date been significant interest in diesel-generated PAHs because of the higher soot and PAH emissions associated with diesel engines [6–8]. Unfortunately, it is difficult to obtain information about diesel in-cylinder PAHs because of the associated high pressure and high temperature environment. The usual approach is to develop predictive numerical models employing detailed PAH mechanisms obtained from canonical systems such as laminar, counterflow diffusion and turbulent diffusion flames [1,9–12]. When applied to diesel engine simulations, these PAH mechanisms are simplified before being incorporated as a part of

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the soot formation model, to minimize the number of scalars required to be resolved in computer simulations [13,14]. However, validation of these PAH models still requires detailed experimental data concerning diesel in-cylinder PAHs. Early experimental studies of diesel in-cylinder PAHs were performed by Ciajolo et al. [15,16], who described the variations in PAHs obtained with increases in the crank angle (CA) by means of a fast sampling valve. The most recent advance in the experimental investigation of diesel in-cylinder PAHs was the laser-induced incandescence technique combined with planar laser-induced fluorescence in an optical diesel engine, which provided data regarding the temporal and spatial evolution of soot and PAHs during the combustion process [17]. Although the studies noted above have provided some interesting results, systematic data on the evolution of in-cylinder PAHs based on quantitative analysis is still limited. In addition, the formation of PAHs in a diesel engine will be affected by fuel identity, such as its aromatic components. Nelson et al. [18] observed that fuels with lower aromatic contents reduced PAH emissions. Mi et al. [19] reported that adding Fluorene to diesel fuel increased the total PAH emissions, while no significant variation in PAH emissions was induced on the addition of toluene. These prior studies, however, have primarily focused on the effects of fuel characteristics on PAH emissions rather than on in-cylinder PAHs.

In this context, the present study explored the evolution of in-cylinder PAHs throughout a diesel engine combustion process fueled with *n*-heptane and the effects of adding toluene to *n*-heptane on in-cylinder PAHs. The resulting data were interpreted in the context of the formation mechanisms of PAHs. Because of the complex compositions of conventional diesel fuel, *n*-heptane was used as a surrogate for the hydrocarbon fuels normally employed in diesel engines. This alkane hydrocarbon has a cetane number close to that of diesel fuel and its oxidation chemistry is very well known. Toluene is often used to simulate the aromatic components of commercial fuels, and so blends of *n*-heptane with toluene were adopted in this work to investigate the effect of adding aromatics on in-cylinder PAHs. The sampling of the in-cylinder PAHs in a direct injection diesel engine was conducted by means of a total cylinder sampling system (TCSS). The PAHs in the samples obtained were analyzed by gas chromatography–mass spectrometry (GC–MS) with programmed temperature vaporization in the solvent vent mode (PTV–SV). The data acquired provides a better understanding of the in-cylinder PAHs generated during actual engine combustion, and should facilitate the development of novel PAH formation models and assist in verifying simulation results.

## 2. Experimental

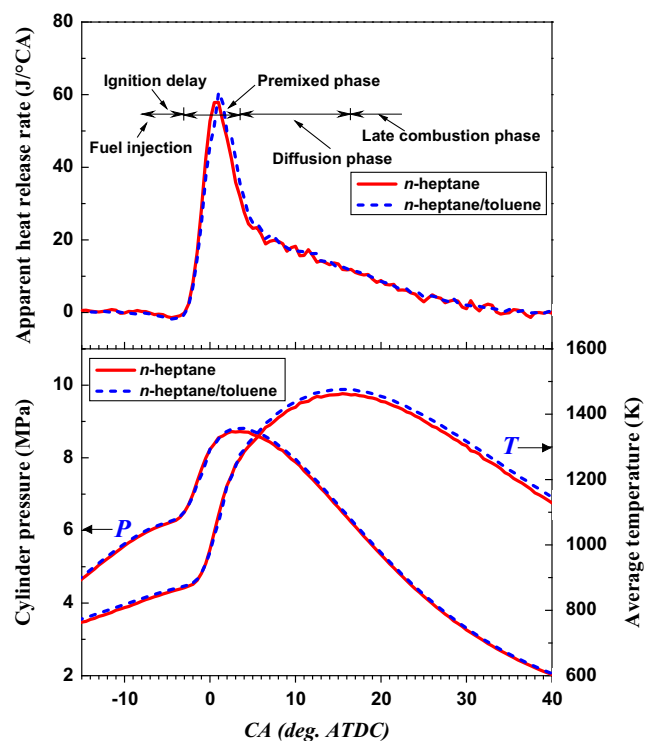
A 5.79 L heavy-duty, direct-injection diesel engine with a bore of 102 mm and a stroke of 118 mm was used in this work. The engine was equipped with a high-pressure, common-rail injection system and a turbocharged/inter-cooled air intake system and powered up to 132 kW at a maximum speed of 2600 rpm. The sixth cylinder was modified to develop a TCSS for use in sampling PAHs from the combustion chamber. In sampling experiments, an aluminum alloy diaphragm was used to seal the engine cylinder head as a sampling valve. At a pre-set CA during a sampling cycle, this

diaphragm was instantaneously cut by an electromagnet-actuated tube cutter, and the cylinder contents were discharged from the cylinder into a sampling bag. Simultaneously, the sampled gas mixture was immediately quenched and diluted by mixing with high pressure nitrogen at a dilution ratio (DR) of 120:1, so as to obtain a temperature below 52 °C and prevent any possible additional reactions during the sampling process. A detailed description of this apparatus and sampling procedure has previously been reported [20–22].

The engine operating conditions are summarized in Table 1. Two diesel fuel surrogates were used: one was *n*-heptane and another was a mixture of 20 vol.% toluene and 80 vol.% *n*-heptane (*n*-heptane/toluene) as a means of ascertaining the effects of aromatic species on the in-cylinder PAHs. Table 2 lists the relevant properties of *n*-heptane and *n*-heptane/toluene. The apparent heat release rate, in-cylinder pressure and average temperature profiles as functions of the CA for each of these two scenarios are shown in

**Table 2**  
Properties of test fuels.

Property	<i>n</i> -Heptane	<i>n</i> -Heptane/toluene
Cetane number	56.0	48.4
H/C	2.28	2.06
Lower heating value (MJ/kg)	44.9	44.0
Density (g/mL, 20 °C)	0.688	0.724



**Fig. 1.** Profiles of apparent heat release rate, in-cylinder pressure and average temperature for *n*-heptane and *n*-heptane/toluene.

**Table 1**  
Operating conditions of the diesel engine.

Fuel	Engine speed (rpm)	Common rail pressure (MPa)	Start of injection (°CA ATDC)	Injection mass (mg)	Injection strategy	Fuel–air equivalence ratio	Intake temperature (K)
<i>n</i> -Heptane	1000	70	–8	21.4	Single	0.267	318
<i>n</i> -Heptane/toluene	1000	70	–8	21.8	Single	0.264	318

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